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Modeling the microstructural evolution during constrained sintering

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Abstract

A mesoscale numerical model able to simulate solid state constrained sintering is presented. The model couples an existing kinetic Monte Carlo (kMC) model for free sintering with a finite element method for calculating stresses. The sintering behavior of a sample constrained by a rigid substrate is simulated, resulting in a larger number of pores near the substrate, which is also observed experimentally.

Introduction

Many applications require components that are sintered under a variety of constraining stresses [1]. Continuum modeling of sintering under constraints has been successfully implemented using different techniques, but linking the macroscopic anisotropic shrinkage to anisotropy in the microstructure is difficult [1]. Here we consider the specific case of the microstructural evolution of a sample sintering on a rigid substrate. Constrained sintering of both metals and ceramics on rigid substrates has been studied experimentally [2-6], and in general, the constrained films had pores perpendicular to the substrate surface and a higher porosity near the substrate. Previously, discrete element method (DEM) simulations [7-8] and surface-evolver simulations [9-10] have been used to simulate constrained sintering at the mesoscale. Here we present a new diffusion-based mesoscale model capable of simulating sintering under constraints. The model couples an existing kinetic Monte Carlo model of sintering [11-12] with a finite element (FE) model to allow for calculation of microstructural stresses during sintering. Coupling an FEM model and a diffusion-based model have previously been attempted in sintering [13-15].

Modeling constrained sintering

In constrained sintering, the stresses present are an additional driving force for sintering and they modify the rates of the diffusive processes in the kMC model. A finite element (FE) model has been implemented and coupled to the existing kMC model, to allow the stresses to be calculated based on events that cause strain in the microstructure. In kMC, densification is driven by annihilation events, which is also the principal process that leads to stress formation. Therefore, grain growth and pore migration are not affected by the stress field. The developed model is a phenomenological model that modifies the probability of annihilation to depend on the compliance (“deformability”) of the microstructure at the place where the annihilation takes place. To simulate this behavior a fixed volumetric force is applied in the FE model at the site where the annihilation event is occurring and its surrounding sites, as shown in Fig. 1. The change in area of the pixels caused by this volumetric contraction is then evaluated in two cases: free sintering, and when the body is constrained. The difference in contraction area is a direct measure of how compliant the local microstructure is to densifications at that point in the sample. This difference in area is then weighted by a tangent hyperbolic function, to calculate the probability that the vacancy will annihilate, as

$$P_{\text{annihilate}} = 1 - \tanh(\alpha(\text{Area}_{\text{constrained}} - \text{Area}_{\text{free}}))$$

This means that the closer a site is to the rigid substrate the less it will contract due to the applied volumetric force, i.e. the harder it will be for the surrounding

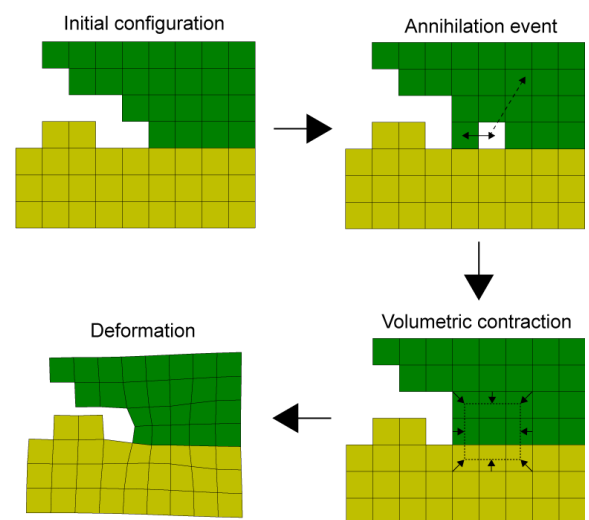


Figure 1: A vacancy site is generated at the grain boundary between two grains and annihilated. This corresponds to a volumetric strain, which causes a deformation of the microstructure.

sites to fill the vacancy formed and to densify the material.

The constant α determines the degree of coupling between the stress field and the microstructural evolution, as shown in Fig. 2. In this model, regions under tension will densify more slowly or not at all. After the FEM calculation, the volumetric strain is assumed to be relaxed before the next Monte-Carlo time step. The calculated stress field is proportional to the chosen volumetric force applied, and therefore the value of volumetric force applied and Young's modulus only influence the value of the coupling constant, α . Poisson's ratio is chosen to be 0.3, which is a typical value for most materials studied in sintering. The model presented here bear resemblance to the inelastic mechanical model introduced in Ref. [16].

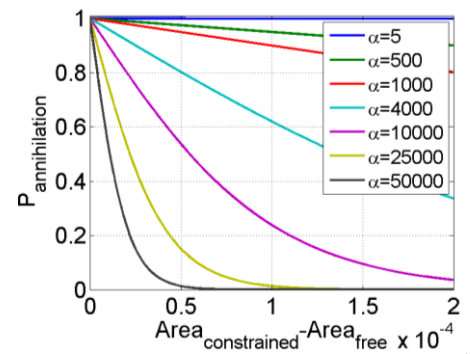


Figure 2: The probability of densification, based on the difference in area due to the volumetric contraction.

The mesh used for the FEM calculation is one bilinear element per pixel. The empty pore sites are not meshed.

Results

The presented results are chosen to show the general validity of the model. We here consider a 2D system, for simplicity. The sintering of a randomly closed packed powder with sample dimensions 600x200 pixels is modeled. The kMC event temperatures are taken to be 0, 0.7 and 1 for grain growth, pore surface diffusion, and vacancy annihilation, respectively, while the attempt frequencies are 0.5, 5 and 1 for the same mechanisms, respectively. Shown in Fig. 3 is the initial microstructure and the microstructure of a sample sintered on a rigid substrate with a strong coupling between the stress field and the microstructure, $\alpha = 25000$. It is seen that the constrained sample has more pores near the substrate, as also seen experimentally. Initially, the relative density is 84.3% and 82.9% near the substrate and near the top of the sample, respectively. After sintering, the relative density has evolved to 85.8% and 94.3%, respectively. The stress field generated by the constraining surface, through the coupling between stress and microstructure, results in this behavior. Anisotropic strain will be discussed in a future work.

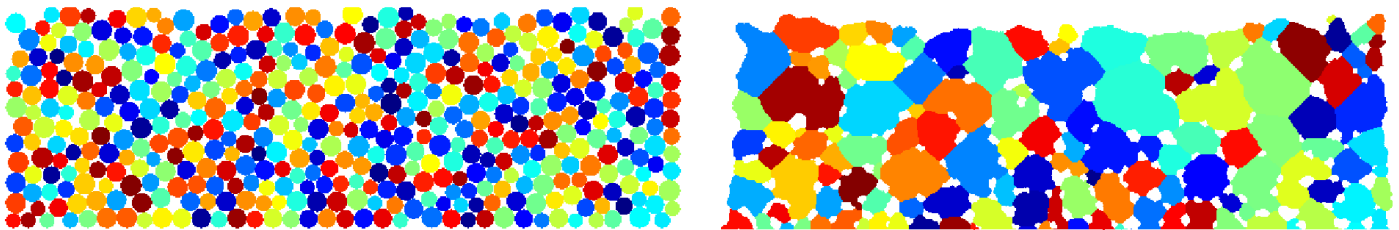


Figure 3: The initial microstructure and the microstructure after sintering, constrained to a surface and with a strong coupling between the stress and the microstructure, $\alpha = 25000$. More pores are clearly seen near the substrate, at the bottom of the sample.

Conclusion

A new microstructural model coupling a kMC and a FE model for modeling constrained sintering is presented. Constrained sintering on a rigid substrate was studied and the model reproduced a larger number of pores near the substrate, as is also observed experimentally.

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